Roles of Defects in Mesoporous 2D Semiconductors for Photocatalytic Applications

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Abstract

In NSRRC, two X-ray techniques, including diffraction (01C2, 09A), absorption (16A, 01C1, 17C1), are employed to reveal crystal and electronic structures of 2D semiconductors. Three types of mesoporous semiconductors (CdSe, S-substituted, Au-decorated ones) are synthesized via solvothermal methods (140 oC) and chemical processes (25-50 oC). Powder X-ray diffraction (PXRD) is a powerful tool to observe structure defects, lattice distortion as well as to estimate coherent lengths of crystalline domains. X-ray absorption techniques (XAS) include XANES and EXAFS that determine oxidation states, coordination numbers and bond distance of targeted active centers (S).

In our study, we are highly interested in heterogeneous catalysis, including hydrogen evolution reaction (HER) and atom transfer radical reaction (ATRA). Photo-induced trions from two electrons and one hole, or vice versa, created in hetrojunctions are photon-sensitizers for effective charge separation as well as radical-initiated chemical reactions. These radicals are generated at S-substituted defect sites in mesoporous CdSe materials. Additionally, the charge separation is rationally assisted by Au-decoration onto the 2D materials with semiconducting properties. PXRD and XAS comfirm existing of structural defects and changing of active-center chemical evironment. NSRRC provides the state-of-the-art facility of X-ray diffraction, absorption techniques that help us to verfity the defects in mesoporous 2D semiconductors.

Keywords – Mesoporous, Defects, 2D Semiconductors, Photocatalytic application

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